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Health and Environmental Effects Profile for Methyl Ethyl Benzenes

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HEALTH AND ENVIRONMENTAL EFFECTS PROFILE FOR METHYL ETHYL BENZENES

ENVIRONMENTAL CRITERIA AND ASSESSMENT OFFICE
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16. ABSTRACT

The Health and Environmental Effects Profile for Methyl Ethyl Benzenes was prepared by the Office of Health and Environmental Assessment, Environmental Criteria and Assessment Office, Cincinnati, OH for the Office of Solid Waste to support listings of hazardous constituents of a wide range of waste streams under Section 3001 of the Resource Conservation and Recovery Act (RCRA). Both published literature and information obtained from Agency program office files were evaluated as they pertained to potential human health, aquatic life and environmental effects of hazardous waste constituents.

Quantitative estimates have been presented provided sufficient data are available. Existing data are insufficient to determine an Acceptable Daily Intake (ADI) or a carcinogenic potency factor for Methyl Ethyl Benzenes.

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PREFACE

Health and Environmental Effects Profiles (HEEPs) are prepared for the Office of Solid Waste by the Office of Health and Environmental Assessment. The HEEPs are intended to support listings of hazardous constituents of a wide range of waste streams under Section 3001 of the Resource Conservation and Recovery Act (RCRA). Both published literature and information obtained from Agency program office files are evaluated as they pertain to potential human health, aquatic life and environmental effects of hazardous waste constituents.

Quantitative estimates are presented provided sufficient data are available. For systemic toxicants, these include, Acceptable Daily Intakes (ADIs) for chronic exposures. An ADI is defined as the amount of a chemical to which humans can be exposed on a daily basis over an extended period of time (usually a lifetime) without suffering a deleterious effect. In the case of suspected carcinogens, ADIs are not estimated in this document series. Instead, a carcinogenic potency factor or q_1^* is provided. These potency estimates are derived for both oral and inhalation exposures where possible. In addition, unit risk estimates for air and drinking water are presented based on inhalation and oral data, respectively.

The first draft of this document was prepared by Syracuse Research Corporation under EPA Contract No. 68-03-3228. The document was subsequently revised after reviews by staff within the Office of Health and Environmental Assessment: Carcinogen Assessment Group, Reproductive Effects Assessment Group, Exposure Assessment Group, and the Environmental Criteria and Assessment Office in Cincinnati.

The HEEPs will become part of the EPA RCRA docket.

ACKNOWLEDGEMENTS

The initial draft of this report was prepared by Syracuse Research Corporation under Contract No. 68-03-3228 for U.S. EPA's Office of Health and Environmental Assessment, Environmental Criteria and Assessment Office, Cincinnati, OH. Dr. Christopher DeRosa was the Technical Project Monitor and Helen Ball was the Project Officer. The final documents in this series were prepared for the Office of Solid Waste, Washington, DC.

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LIST OF ABBREVIATIONS

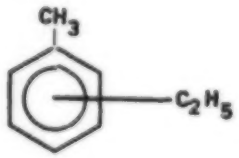
CNS	Central nervous system
EC_{50}	Median effective concentration
GC/MS	Gas chromatography/mass spectrometry
LD_{Lo}	Lowest lethal dose
ppb	Parts per billion
ppm	Parts per million
TLV	Threshold limit value

1. INTRODUCTION

1.1. STRUCTURE AND CAS NUMBER

Methylethylbenzene is also known as ethyltoluene and ethylmethylbenzene. 1-Ethyl-2-methylbenzene is also known as o-ethyltoluene, 2-ethyltoluene, o-methylethylbenzene and o-ethylmethylbenzene. 1-Ethyl-3-methylbenzene is also known as m-ethyltoluene, 3-ethyltoluene, m-methylethylbenzene and m-ethylmethylbenzene. 1-Ethyl-4-methylbenzene is also known as p-ethyltoluene, 4-ethyltoluene, p-methylethylbenzene and p-ethylmethylbenzene. 4-Ethyl-1,2-dimethylbenzene is also known as 4-ethyl-o-xylene; 2-methyl-4-ethyltoluene; 1,2-dimethyl-4-ethylbenzene; and 1-ethyl-3,4-dimethylbenzene. The structures of these compounds are shown below:

<u>Ethyltoluene</u>

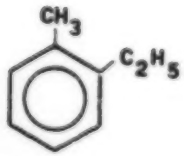


Molecular formula: C_9H_{12}

Molecular weight: 120.12

Chemical Abstracts Services (CAS) Registry Number: 25550-14-5.

<u>o-ethyltoluene</u>

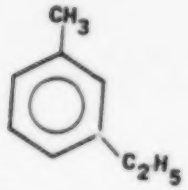


Molecular formula: C_9H_{12}

Molecular weight: 120.12

Chemical Abstracts Services (CAS) Registry Number: 611-14-3

m-ethyltoluene



Molecular formula: C_9H_{12}

Molecular weight: 120.12

Chemical Abstracts Service (CAS) Registry Number: 620-14-4

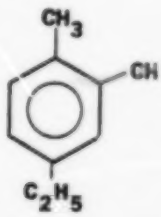
p-ethyltoluene

Molecular formula: C_9H_{12}

Molecular weight: 120.12

Chemical Abstracts Services (CAS) Registry Number: 622-96-8

4-ethyl-o-xylene



Molecular formula: $C_{10}H_{14}$

Molecular weight: 134

Chemical Abstracts Services (CAS) Registry Number: 934-80-5

1.2. PHYSICAL AND CHEMICAL PROPERTIES

The o-, m- and p-isomers of ethyltoluene are colorless liquids at ambient conditions. 4-Ethyl-o-xylene is also a colorless liquid at ambient conditions.

Some of the physical and chemical properties of these compounds are given in Table 1-1 [Chemical Rubber Company (CRC, 1980)].

1.3. PRODUCTION DATA

Ethyltoluene was produced in 1982 by Dow Chemical, Midland, MI [Stanford Research Institute (SRI, 1983)]. The volume of production was not provided. In 1977, 0.1-1 million pounds of o-ethyltoluene was produced by Koppers, Follansbee, WV; an unstated volume of p-ethyltoluene was produced by Mobil Research and Development, Paulsboro, NJ, and 1-10 million pounds of 4-ethyl-o-xylene were produced by SPPC, Nueces, TX (U.S. EPA, 1983).

Ethyltoluene is produced by the alkylation of toluene. Enrichment of the yield of the o-, m- or p-isomer can be accomplished by varying the reaction condition [Capital Systems Group (CSG and Dynamac, 1982)].

1.4. USE DATA

These compounds are used as solvents and in chemical synthesis, and can be found in gasoline (CSG and Dynamac, 1982).

TABLE 1-1

Physical and Chemical Properties of the Methyl Ethyl Benzenes*

Compound	Boiling Point	Melting Point	Density (at 20°C)	Vapor Pressure
2-ethyltoluene	165.2°C	-80.8°C	0.8807	1 mm Hg at 9.4°C
3-ethyltoluene	161.3°C	-95.5°C	0.8645	1 mm Hg at 7.2°C
4-ethyltoluene	162°C	-62.3°C	0.8614	1 mm Hg at 7.6°C
4-ethyl-o-xylene	189.7°C	-67°C	0.8745	NR

*Source: CRC, 1980

NR = Not reported

2. ENVIRONMENTAL FATE AND TRANSPORT PROCESSES

Based on production, use and monitoring data (Sections 1.3., 1.4. and Chapter 3), ethyltoluene isomers may enter the environment from petroleum spills, automobile exhaust, refineries, chemical plants and automobile painting shops. Relatively high vaporization of the ethyltoluenes may be predicted by virtue of their high vapor pressure (>1 mm Hg at ambient temperature and their low water solubility). Smith and Harper (1982) reported a moderate volatilization rate from water for m-ethyltoluene, based on an observed average ratio of component volatilization rate constant/oxygen reaeration rate constant (K_v^c/K_v^o) of ~0.53.

Lloyd et al. (1976) estimated rate constants for the disappearance of o-ethyltoluene, m-ethyltoluene and p-ethyltoluene from an environmental chamber under simulated atmospheric conditions (1 atmosphere, 305°K) of 1.4, 1.9 and 1.3×10^{-11} cm^3 $molecule^{-1}$ sec^{-1}, respectively. If one assumes that OH• radicals are responsible for the depletion of the compounds, and that the typical average atmospheric concentration of OH• radicals is 1×10^6 molecules cm^{-3} (Logan et al., 1981), then the calculated lifetimes of o-ethyltoluene, m-ethyltoluene and p-ethyltoluene in the atmosphere are 20, 15 and 21 hours, respectively.

Using the same rate constants and assuming an atmospheric concentration of OH• radicals of 1×10^7 molecules cm^{-3} for polluted air, Darnall et al. (1976) predicted atmospheric lifetimes of the o-, m- and p-ethyltoluenes of 1.5-2.1 hours.

Kunz and Chapman (1981) reported the microbial oxidation of the ethyltoluenes by certain strains of Pseudomonas putida. Good growth of 5/7 strains of P. putida was observed when m-ethyltoluene was used as a substrate. Slight growth of 2/7 strains on p-ethyltoluene and no growth in any of 7 strains on o-ethyltoluene were also observed. The metabolic pathway of

the substrates was postulated to be a single step oxidation of methyl group to form the corresponding benzoic acid.

Kappeler and Wuhrmann (1978) observed the biodegradation of all title compounds by the autochthonous microflora found in groundwater. An aqueous solution of hydrocarbons was prepared by shaking 1 mℓ of gas oil [a liquid petroleum distilled with a boiling range of 450-800°F (Hawley, 1977)] with 1 ℓ of groundwater and discarding the oil phase. The aqueous solution, containing ~2 ppm hydrocarbons, was allowed to circulate through a percolation column containing quartz sand for up to 192 hours. Samples of the percolate were withdrawn at intervals and were analyzed with GC/MS. No significant decrease in hydrocarbon concentration of the percolate was observed during a lag phase of 120 hours, but all title compounds were undetectable by 192 hours after equilibration.

Van der Linden (1978) reported the microbial oxidation of all title compounds by seawater. An aqueous solution of hydrocarbons, prepared by mixing 100 mℓ of gas oil with 1 ℓ of artificial seawater, was inoculated with North Sea coast water and incubated for 10 days at 20°C with or without the addition of a bacterial inhibitor. The concentration of o-ethyltoluene decreased from 16.8 to 0.2 µg/ℓ without bacterial inhibition. Similarly, the concentration of m-ethyltoluene decreased from 23.3 to 0.4 µg/ℓ, p-ethyltoluene decreased from 11.0 to 0.4 µg/ℓ, and 4-ethyl-o-xylene decreased from 12.5 to 0.4 µg/ℓ. When a bacterial inhibitor was present during the 10-day incubation, no diminution of the original concentrations of the title compounds was observed. All compounds were identified and measured with high resolution gas-liquid chromatography.

Pertinent data regarding the fate of the methylethylbenzenes in soil were not located in the available literature (see Appendix).

3. EXPOSURE

Ethyltoluene has been detected in ambient air. Its presence has been attributed to several sources, especially engine exhaust (GSC and Dynamac, 1982). Levels of mixed ethyltoluene in downtown Los Angeles and Azusa, California, air samples have been reported to be 7.5 and 3.0 ppb, respectively (Altshuller et al., 1971). Air samples near Houston, Texas, have been reported to contain 1.5-4.0 ppb of mixed ethyltoluene (Bertsch et al., 1974). Mean p-ethyltoluene levels in air measured over a 12-day period in April-July, 1979, at Los Angeles, California, Phoenix, Arizona and Oakland, California, were reported to be 1.5 ppb (range = 0.10-10.15), 1.5 ppb (range = 0.20-7.37) and 0.66 ppb (range = 0.02-3.40), respectively (Singh et al., 1981). Air samples above Lake Michigan have been reported to contain 0.3 ppb of the m- and p-isomers of ethyltoluene (Miller and Alkezweeny, 1980). Airborne levels of the o-, m- and p-isomers of ethyltoluene downwind of a Jamesville, Michigan, automobile plant were reportedly 2.0-2.5, 1.5 and 1.0-2.0 $\mu g/m^3$, respectively (Sexton and Westburg, 1980).

Petersson (1982) measured airborne levels of all four title compounds near a Saab plant, 1 km downwind from a Volvo plant, and in a remote city. The concentration of o-ethyltoluene at these sites was 30, 5.6 and 0.05 $\mu g/m^3$, respectively. The concentration of m-ethyltoluene at the above sites was 71, 10.3 and 0.1 $\mu g/m^3$, respectively. The concentrations of p-ethyltoluene at the above sites were 32, 4.3 and 0.04 $\mu g/m^3$, respectively. The concentrations of 4-ethyl-o-xylene at the above sites were 9.9, 2.9 and 0.01 $\mu g/m^3$, respectively.

The ethyltoluenes have been detected in drinking water and in sea, river and groundwater. Three carbon-substituted alkylbenzenes (including ethyltoluene and propylbenzene) were detected at levels between 0.01-2.4 $\mu g/\ell$

in samples from three New Orleans drinking water plants (Keith et al., 1976). o- and m-Ethyltoluene have been detected at 0.02-0.05 µg/ℓ in samples from drinking water plants at Jefferson Parish, LA (CSC and Dynamac, 1982). Gschwend et al. (1982) and Mantoura et al. (1982) reported detecting mixed m- and p-ethyltoluene in samples of seawater at a mean concentration of 5.7 ng/ℓ(range 1.4-17 ng/ℓ) from a dock at Vineyard Sound, Massachusetts. Zoeteman et al. (1980) reported a concentration of 0.01 µg o-ethyltoluene/ℓ in the Lobith/Gorinchem river system in Holland. Steurmer et al. (1982) reported detecting all four title compounds in samples of water taken from 3 water wells, each drilled near a burn cavity wherein underground coal gasification had occurred 3 months earlier. The range of o-ethyltoluene, m-ethyltoluene, p-ethyltoluene and 4-ethyl-o-xylene isomers measured was 61-220, 45-250, 31-140 and 15-49 ppb, respectively.

Montz et al. (1982) reported detecting o-, m- and p-ethyltoluene in a 160 ℓ container of water in which a 7 or 10 horsepower outboard motor was operated for 30 minutes. The concentrations of o- and m-, and p-ethyltoluene in water from the 7 horsepower motor were 1 and 2.5 ppm, respectively. The concentrations of o- and m-, and p-ethyltoluene in water from the 10 horsepower motor were 3.7 and 9.3 ppm, respectively. The inefficient design of 2-cycle outboard motors allows a wide variety of organic compounds to be released into water.

Hiatt (1983) detected m-ethyltoluene (40 ppb) and 4-ethyl-o-xylene (9 ppb) in samples of tissues from rainbow trout of unknown origin. A sample of carp (unknown origin) contained 130 ppb of m-ethyltoluene.

4. PHARMACOKINETICS

Chin et al. (1980, 1981) have investigated the absorption, distribution, metabolism and excretion of a mixture of ^{14}C-ring labeled o-, m- and p-ethyltoluene isomers (1:2:1) in male Harlan-Wistar rats (100-120 g, 3/group). The animals were exposed to atmospheres containing ~1 mg ethyltoluene/ℓ for 6 hours. Each rat absorbed ~19 mg of compound. Assuming a respiratory rate of 100 mℓ/minute, each rat was exposed to 36 mg of ethyltoluene, resulting in an absorption efficiency of 53%. The relative absorption efficiencies of the three isomers were not determined.

After 48 hours, 0.3% of the absorbed dose remained in the animals. The highest amounts were found in the carcass (0.120%), gastrointestinal tract (0.102%), liver (0.068%) and plasma (0.010%). The authors did not determine the time-course for distribution to and absorption by the various tissues.

Seven metabolites, labeled A, B, C, D, E, F and G were found in the urine. These accounted for 0.8, 34.9, 29.1, 31.1, 2.1, 1.2 and 0.8% of the total metabolites, respectively. Under the same conditions, female beagle dogs produced qualitatively the same metabolites; however, only trace amounts of metabolites F and G were present in dog urine. These metabolites were also produced by liver explants from both species, except that dog liver did not produce metabolite E *in vitro*. No structural identification was attempted for any of the metabolites.

The excretion of ^{14}C was measured in urine, feces and expired air. Excretion was essentially complete within 48 hours. Urinary excretion accounted for the majority of the absorbed dose (71.5%) with minor amounts excreted in the feces (2.7%) and expired air (0.25% CO_2, 1.3% other). Excretory products and tissue residues accounted for 76.1±26.3% of the

absorbed dose. The large standard derivation was due to the variability in the urinary excretion data. The authors offered no explanation for the poor reproducibility of these data.

5. EFFECTS

5.1. CARCINOGENICITY

Pertinent data regarding the carcinogenicity of ethyltoluenes were not located in the available literature. These compounds are not scheduled for testing by the National Toxicology Program (NTP, 1983).

5.2. MUTAGENICITY

Pertinent data regarding the mutagenicity of ethyltoluene isomers were not located in the available literature.

5.3. TERATOGENICITY

Pertinent data regarding the teratogenicity of the ethyltoluenes were not located in the available literature. Dimethylethylbenzene was identified in the maternal and cord blood of a normal woman at the time of delivery; however, the biologic significance of this observation is not clear (Dowty et al., 1976).

5.4. OTHER REPRODUCTIVE EFFECTS

Pertinent data regarding other reproductive effects of the ethyltoluenes were not located in the available literature.

5.5. CHRONIC AND SUBCHRONIC TOXICITY

Pertinent data regarding the chronic or subchronic toxicity of the ethyltoluenes were not located in the available literature.

5.6. OTHER RELEVANT INFORMATION

Sandmeyer (1981) stated that the toxicities of ethyltoluenes resemble those of ethylbenzene. No data were presented to support this conclusion. The National Institute for Occupation Safety and Health (NIOSH), 1983 reports oral LD_{Lo} values of 5000 mg/kg for o- and p-ethyltoluene in rats. In a review, Sandmeyer (1981) states that exposure to 3000 ppm ethyltoluene vapors resulted in a loss of the righting reflex in mice; however, the

reference cited does not appear to have any bearing on ethyltoluene toxicity (Kojima and Kobayashi, 1973).

Furnas and Hine (1958) exposed eight male Long-Evans rats to atmospheres containing 4000 ppm p-ethyltoluene. Each rat received five 25-minute exposures during 1 day. This treatment resulted in 50% mortality, local irritation, depression and quivering or twitching, but no convulsions. No gross lesions, other than those attributable to local irritation of the respiratory tract, were observed at necropsy. Microscopic examination did not reveal any specific damage to the CNS.

6. AQUATIC TOXICITY

6.1. ACUTE TOXICITY

Pertinent data regarding the toxic effects of acute exposure to ethyltoluenes on aquatic animals were not located in the available literature.

6.2. CHRONIC EFFECTS

Pertinent data regarding the effects of chronic ethyltoluene exposure on aquatic organisms were not located in the available literature.

6.3. PLANT EFFECTS

The concentration of o- and p-ethyltoluene required to cause a 50% reduction in photosynthetic rate (EC_{50}) determined by radiolabeled-carbon uptake was determined in Chlorella vulgaris and Chlamydomonas angulosa (Hutchinson et al., 1979). For C. vulgaris, the EC_{50} values for both isomers were $\sim 7 \times 10^{-4}$ M (0.84 mg/ℓ). Para-ethyltoluene was slightly more toxic to C. angulosa than was the ortho-isomer, with EC_{50} values of 6.5×10^{-4} M (0.78 mg/ℓ) and 9.2×10^{-4} M (1.1 mg/ℓ), respectively.

6.4. RESIDUE

Rainbow trout taken below Hoover Dam on the Colorado River were reported to contain 40 ppb (ng/g tissue on a wet weight basis) m-ethyltoluene. Carp collected in the Las Vegas Wash contained 130 ppb (ng/g tissue) of m-ethyltoluene (Hiatt, 1983).

6.5. OTHER RELEVANT INFORMATION

Additional data pertinent to the aquatic toxicity of the ethyltoluenes were not located in the available literature.

7. EXISTING GUIDELINES AND STANDARDS

7.1. HUMAN

No existing guidelines or standards were located in the available literature. TLVs have not been established by the American Conference of Governmental Industrial Hygienists (ACGIH, 1980, 1982).

7.2. AQUATIC

Guidelines and standards for the protection of aquatic organisms from the toxic effects of ethyltoluenes were not located in the available literature.

8. RISK ASSESSMENT

No data regarding the potential carcinogenicity, mutagenicity, teratogenicity, reproduction toxicity or chronic toxicity of the ethyltoluenes was located in the available literature (see Appendix). Acute inhalation experiments indicate that ethyltoluenes are CNS depressants (Sandmeyer, 1981; Furnas and Hine, 1958). An oral LD_{Lo} in rats of 5000 mg/kg has been reported for o-ethyltoluene and for p-ethyltoluene (NIOSH, 1983), indicating that these compounds have a relatively low oral toxicity.

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APPENDIX: LITERATURE SEARCHED

This profile is based on data identified by computerized literature searches of:

CA SEARCH (Files 308, 309, 310, 311, 320)
TOXLINE
MEDLINE
RTECS
SCI SEARCH
CHM TADS
STORET
SRC Environmental Fate Data Bases
SANSS
AQUIRE

Most of these searches were conducted in May, 1983. In addition, hand searches were made of Chemical Abstracts (Collective Indices 6, 7 and 8th), and the following secondary sources were reviewed:

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